

26/11/2004

10809125

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PASSWORD:

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* * * * * Welcome to STN International * * * * *

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NEWS 3 SEP 01 INPADOC: New family current-awareness alert (SDI) available
NEWS 4 SEP 01 New pricing for the Save Answers for SciFinder Wizard within
STN Express with Discover!
NEWS 5 SEP 01 New display format, HITSTR, available in WPIDS/WPINDEX/WBIX
NEWS 6 SEP 27 STANDARDS will no longer be available on STN
NEWS 7 SEP 27 SWETSCAN will no longer be available on STN
NEWS 8 OCT 28 KOREAPAT now available on STN
NEWS 9 NOV 18 Current-awareness alerts, saved answer sets, and current
search transcripts, to be affected by CERAB, COMPUAB, ELCOM,
and SOLIDSTATE reloads

NEWS EXPRESS OCTOBER 29 CURRENT WINDOWS VERSION IS V7.01A, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
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result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 19:23:14 ON 26 NOV 2004

=> FILE REG

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 19:23:22 ON 26 NOV 2004

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 24 NOV 2004 HIGHEST RN 788132-72-9
DICTIONARY FILE UPDATES: 24 NOV 2004 HIGHEST RN 788132-72-9

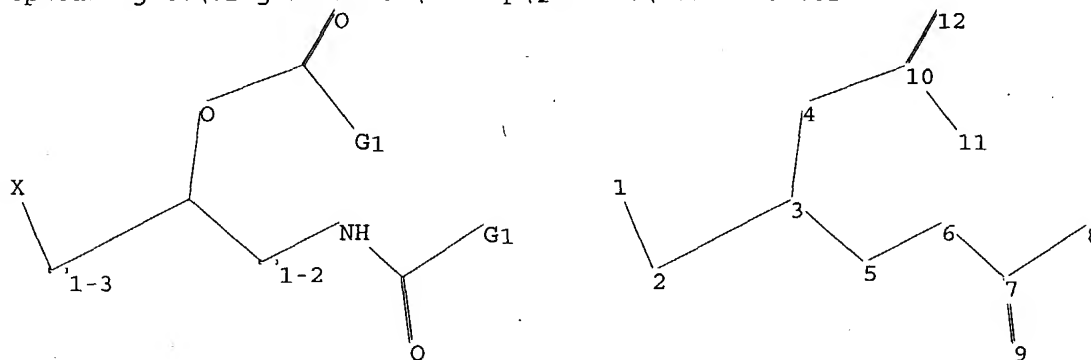
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>
Uploading C:\Program Files\Stnexp\Queries\10809125.str



chain nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
1-2 2-3 3-4 3-5 4-10 5-6 6-7 7-8 7-9 10-11 10-12
exact/norm bonds :
3-4 4-10 5-6 6-7 7-8 7-9 10-11 10-12
exact bonds :
1-2 2-3 3-5

G1:CF2,CF3,CCl2,CCl3,CBr2,CBr3

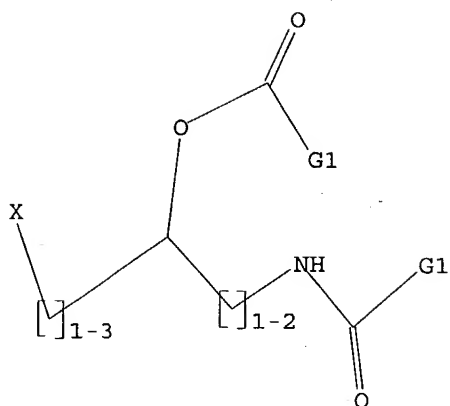
Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS

L1 STRUCTURE UPLOADED

=> D
L1 HAS NO ANSWERS
L1 STR

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10809125



G1 CF2,CF3,CCl2,CCl3,CBr2,CBr3

Structure attributes must be viewed using STN Express query preparation.

=> S L1 FULL

FULL SEARCH INITIATED 19:23:50 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 2175 TO ITERATE

100.0% PROCESSED 2175 ITERATIONS

9 ANSWERS

SEARCH TIME: 00.00.01

L2 9 SEA SSS FUL L1

=> FILE CAPLUS

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

155.42

155.63

FILE 'CAPLUS' ENTERED AT 19:23:56 ON 26 NOV 2004

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FILE COVERS 1907 - 26 Nov 2004 VOL 141 ISS 23

FILE LAST UPDATED: 25 Nov 2004 (20041125/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> S L2

26/11/2004

10809125

L3

2 L2

=> D IBIB ABS HITSTR TOT

26/11/2004

10809125

L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:832754 CAPLUS

DOCUMENT NUMBER: 137:337876

TITLE: Preparation of pharmaceutically active (S)-2-oxo-5-oxazolidinylmethylacetamides via a one step process from (S)-acetamidoacetoxypyrans and N-aryl-O-alkylcarbamates

INVENTOR(S): Berrault, William R.; Pearlman, Bruce A.; Godrej, Debara D.

PATENT ASSIGNEE(S): Pharmacia & Upjohn Company, USA

SOURCE: PCT Int. Appl., 30 pp.

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

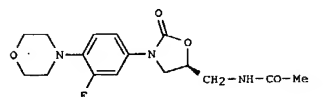
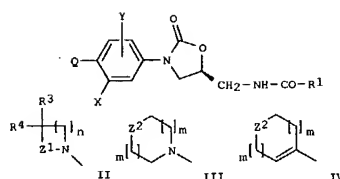
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002085849	A2	20021031	WO 2002-US8261	20020415
WO 2002085849	A3	20030306		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2002169312	A1	20021114	US 2002-122852	20020415
US 2004220407	A1	20041104	US 2004-809125	20040325
PRIORITY APPLN. INFO.: US 2001-285586P P 20010420				
US 2002-365581P P 20020319				
US 2002-122852 A3 20020415				

OTHER SOURCE(S):
GI

CASREACT 137:337876; MARPAT 137:337876

L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

(Continued)



AB Title compds. I [X, Y = H, F; Q = II, III, IV, etc. or Q and X together = dihydropyrrolidine (un)substituted with R5; R1 = CH3 optionally substituted by 1-3 F or Cl atoms; R3 = H, CH3; R4 = H, OH, alkyl, etc.;

R5 = COCH3, CHO, COCHCl2, etc.; Z1 = CH2(CH2)p, CH(OH)(CH2)p, CO; Z2 = S, SO2, etc.; m = 0-1; n = 1-3; p = 0-2] were prepd via a one step process from (S)-acetamidoacetoxypyrans and N-aryl-O-alkylcarbamates. For example, to a solution of N-carbobenzoxy-3-fluoro-4-morpholinylaniline (3.125 mmol) in DMF (2.0 mL) and MeOH (6.32 mmol) was added a solution of lithium tert-butoxide in THF (9.39 mmol), while keeping the reaction temperature less than 25 °C with an ice bath. The solution was cooled to 5 °C and (S)-N-[2-(acetoxy)-3-chloropropyl]acetamide (6.234 mmol) added in one portion. The reaction was allowed to stand for 21 h at 21 °C, then quenched with saturated aqueous NH4Cl (5.0 mL), H2O (30 mL), brine (20 mL) and CH2Cl2 (20 mL). The organic layer was separated, the aqueous phase washed with CH2Cl2 (3 X 20 mL) and the combined CH2Cl2 fractions dried over anhydrous Mg2SO4 and concentrated in vacuo to an oil. The residue was dissolved in xylenes (25 mL), followed by vacuum filtration of the crystalline material to provided oxazolidinylmethylacetamide V in 61.8 % yield. A key-step of the process is the in situ generation of (S)-N-oxiranylmethylacetamide, which is an unstable chiral epoxide that can not be isolated on large scale by the prior art. Approx. 5-specific claimed examples of I and one

L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

intermediate were prepd.

IT 474021-98-2P 474021-99-3P 474022-02-1P

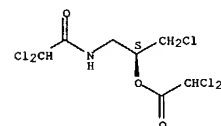
474022-03-2P 474022-05-4P 474022-06-5P

RL: IMP (Industrial manufacture); RCT (Reactant); SPM (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate: preparation of oxazolidinylmethylacetamides via a one step process from N-aryl-O-alkylcarbamates and acetamidoacetoxypyrans)

RN 474021-98-2 CAPLUS

CN Acetic acid, dichloro-, (1S)-2-chloro-1-[(dichloroacetyl)amino]methyl]ethyl ester (9CI) (CA INDEX NAME)

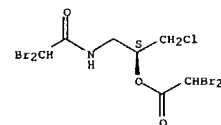
Absolute stereochemistry.



RN 474021-99-3 CAPLUS

CN Acetic acid, dibromo-, (1S)-2-chloro-1-[(dibromoacetyl)amino]methyl]ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

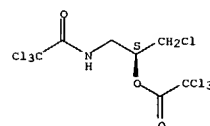


RN 474022-02-1 CAPLUS

CN Acetic acid, trichloro-, (1S)-1-(chloromethyl)-2-[(trichloroacetyl)amino]ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

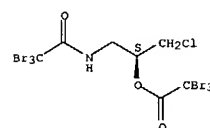
L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 474022-03-2 CAPLUS

CN Acetic acid, tribromo-, (1S)-1-(chloromethyl)-2-[(tribromoacetyl)amino]ethyl ester (9CI) (CA INDEX NAME)

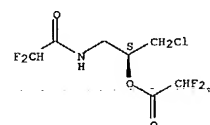
Absolute stereochemistry.



RN 474022-05-4 CAPLUS

CN Acetic acid, difluoro-, (1S)-2-chloro-1-[(difluoroacetyl)amino]methyl]ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 474022-06-5 CAPLUS

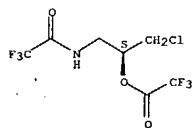
CN Acetic acid, trifluoro-, (1S)-1-(chloromethyl)-2-[(trifluoroacetyl)amino]ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1975:514272 CAPLUS

DOCUMENT NUMBER: 83:114272

TITLE: Reactions of amino acids with trifluoroacetic anhydride. III. 41-Substituted 2-trifluoromethyl-4-(3,3,3-trifluoro-2-trifluoroacetoxypropylidene)-2-oxazolin-5-ones

AUTHOR(S): Austel, Volkhard; Stiglich, Wolfgang
CORPORATE SOURCE: Org.-Chem. Inst., Tech. Univ. Berlin, Berlin, Fed. Rep. Ger.

SOURCE: Chemische Berichte (1975), 108(7), 2361-7
CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 83:114272

GI For diagram(s), see printed CA issue.
AB Enol trifluoroacetates I (R = H, Me, Et, Ph) rearrange to the title compds. II on heating in MeCN. The stereochem. and mechanism of the reaction are discussed. Addition of MeOH to 4-ethylideneoxazolinone III gave

2-methoxyoxazolinone IV.

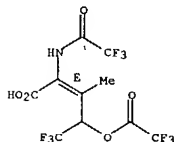
IT 56945-42-7P 57002-47-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

RN 56945-42-7 CAPLUS

CN 2-Pentenoic acid, 5,5,5-trifluoro-3-methyl-2-[(trifluoroacetyl)amino]-4-[(trifluoroacetyl)oxy]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

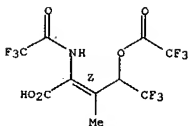


RN 57002-47-8 CAPLUS

CN 2-Pentenoic acid, 5,5,5-trifluoro-3-methyl-2-[(trifluoroacetyl)amino]-4-[(trifluoroacetyl)oxy]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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=> LOGOFF

ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF

LOGOFF? (Y)/N/HOLD:Y

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
9.96	165.59

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-1.40	-1.40

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STN INTERNATIONAL LOGOFF AT 19:24:17 ON 26 NOV 2004